Problem 7 (30 Points)

Data-driven field prediction models can be used as a substitute for performing expensive calculations/simulations in design loops. For example, after being trained on finite element solutions for many parts, they can be used to predict nodal von Mises stress for a new part by taking in a mesh representation of the part geometry.

Consider the plane-strain compression problem shown in "data/plane-strain.png".

In this problem you are given node features for 100 parts. These node features have been extracted by processing each part shape using a neural network. You will perform feature selection to determine which of these features are most relevant using feature selection tools in sklearn.

You are welcome to use any of the code provided in the lecture activities.

Summary of deliverables:

SciKit-Learn Models: Print Train and Test MSE

- `LinearRegression()` with all features
- `DecisionTreeRegressor()` with all features
- `LinearRegression()` with features selected by `RFE()`
- `DecisionTreeRegressor()` with features selected by `RFE()`

Feature Importance/Coefficient Visualizations

- Feature importance plot for Decision Tree using all features
- Feature coefficient plot for Linear Regression using all features
- Feature importance plot for DT showing which features RFE selected
- Feature coefficient plot for LR showing which features RFE selected

Stress Field Visualizations: Ground Truth vs. Prediction

- Test dataset shape index 8 for decision tree and linear regression with all features
- Test dataset shape index 16 for decision tree and linear regression with RFE features

Questions

- Respond to the 5 prompts at the end

Imports and Utility Functions:

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.tree import DecisionTreeRegressor
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
from sklearn.feature_selection import RFE

def plot_shape(dataset, index, model=None, lims=None):
    x = dataset["coordinates"][index][:,0]
    y = dataset["coordinates"][index][:,1]

    if model is None:
        c = dataset["stress"][index]
    else:
        c = model.predict(dataset["features"][index])

    if lims is None:
        lims = [min(c),max(c)]

    plt.scatter(x,y,s=5,c=c,cmap="jet",vmin=lims[0],vmax=lims[1])
    plt.colorbar(orientation="horizontal", shrink=.75, pad=0,ticks=lims)
    plt.axis("off")
    plt.axis("equal")

def plot_shape_comparison(dataset, index, model, title=""):
    plt.figure(figsize=[6,3.2], dpi=120)
    plt.subplot(1,2,1)
    plot_shape(dataset,index)
    plt.title("Ground Truth",fontsize=9,y=.96)
    plt.subplot(1,2,2)
    c = dataset["stress"][index]
    plot_shape(dataset, index, model, lims = [min(c), max(c)])
    plt.title("Prediction",fontsize=9,y=.96)
    plt.suptitle(title)
    plt.show()

def load_dataset(path):
    dataset = np.load(path)
```

```python
    coordinates = []
    features = []
    stress = []
    N = np.max(dataset[:,0].astype(int)) + 1
    split = int(N*.8)
    for i in range(N):
        idx = dataset[:,0].astype(int) == i
        data = dataset[idx,:]
        coordinates.append(data[:,1:3])
        features.append(data[:,3:-1])
        stress.append(data[:,-1])
    dataset_train = dict(coordinates=coordinates[:split], features=features[:split], stress=stress[:split])
    dataset_test = dict(coordinates=coordinates[split:], features=features[split:], stress=stress[split:])
    X_train, X_test = np.concatenate(features[:split], axis=0), np.concatenate(features[split:], axis=0)
    y_train, y_test = np.concatenate(stress[:split], axis=0), np.concatenate(stress[split:], axis=0)
    return dataset_train, dataset_test, X_train, X_test, y_train, y_test

def get_shape(dataset,index):
    X = dataset["features"][index]
    y = dataset["stress"][index]
    return X, y

def plot_importances(model, selected = None, coef=False, title=""):
    plt.figure(figsize=(6,2),dpi=150)
    y = model.coef_ if coef else model.feature_importances_
    N = 1+len(y)
    x = np.arange(1,N)

    plt.bar(x,y)

    if selected is not None:
        plt.bar(x[selected],y[selected],color="red",label="Selected Features")
        plt.legend()

    plt.xlabel("Feature")

    plt.ylabel("Coefficient" if coef else "Importance")
    plt.xlim(0,N)
    plt.title(title)
    plt.show()
```

Loading the data

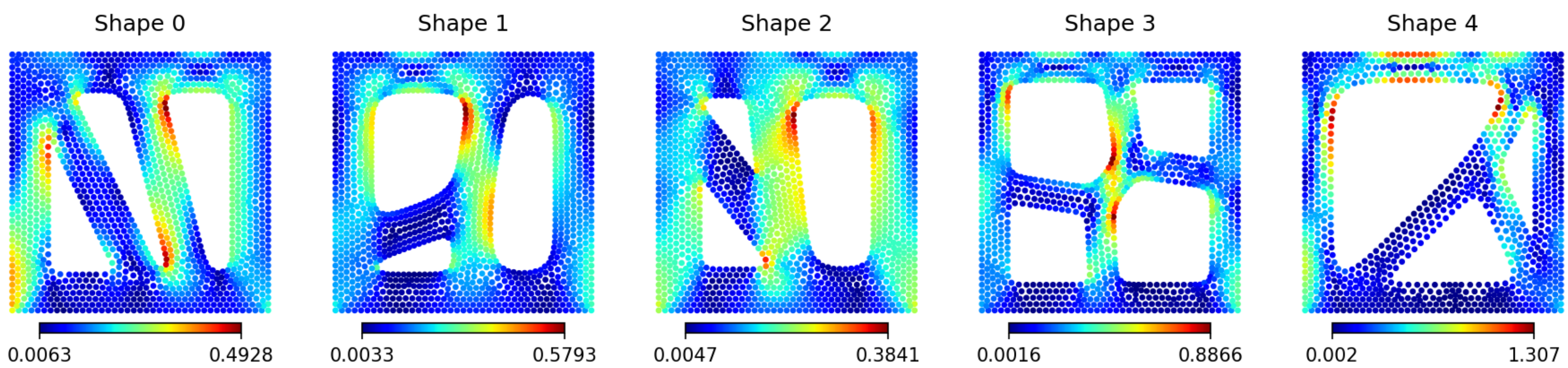
First, complete the code below to load the data and plot the von Mises stress fields for a few shapes.
You'll need to input the path of the data file, the rest is done for you.

All training node features and outputs are in `X_train` and `y_train`, respectively. Testing nodes are in `X_test`, `y_test`.

`dataset_train` and `dataset_test` contain more detailed information such as node coordinates, and they are separated by shape. Get features and outputs for a shape by calling `get_shape(dataset,index)`. `N_train` and `N_test` are the number of training and testing shapes in each of these datasets.

In [2]:
```
# YOUR CODE GOES HERE
# Define data_path
data_path = 'data/stress_nodal_features.npy'
dataset_train, dataset_test, X_train, X_test, y_train, y_test = load_dataset(data_path)
N_train = len(dataset_train["stress"])
N_test = len(dataset_test["stress"])

plt.figure(figsize=[15,3.2], dpi=150)
for i in range(5):
    plt.subplot(1,5,i+1)
    plot_shape(dataset_train,i)
    plt.title(f"Shape {i}")
plt.show()
```



Fitting models with all features

Create two models to fit the training data `X_train`, `y_train`:

1. A `LinearRegression()` model
2. A `DecisionTreeRegressor()` model with a `max_depth` of 20

Print the training and testing MSE for each.

In [14]:
```
# YOUR CODE GOES HERE
model_lr = LinearRegression()
model_lr.fit(X_train,y_train)
pred_train_lr = model_lr.predict(X_train)
pred_test_lr = model_lr.predict(X_test)
print("Mean squared error for Linear Regression model for the training set:",
      mean_squared_error(y_train,pred_train_lr))
print("Mean squared error for Linear Regression model for the testing set:",
      mean_squared_error(y_test,pred_test_lr))

model_dt = DecisionTreeRegressor(max_depth = 20)
model_dt.fit(X_train,y_train)
pred_train_dt = model_dt.predict(X_train)
pred_test_dt = model_dt.predict(X_test)
print("Mean squared error for Decision Tree Regressor model for the training set:",
      mean_squared_error(y_train,pred_train_dt))
print("Mean squared error for Decision Tree Regressor model for the testing set:",
      mean_squared_error(y_test,pred_test_dt))
```

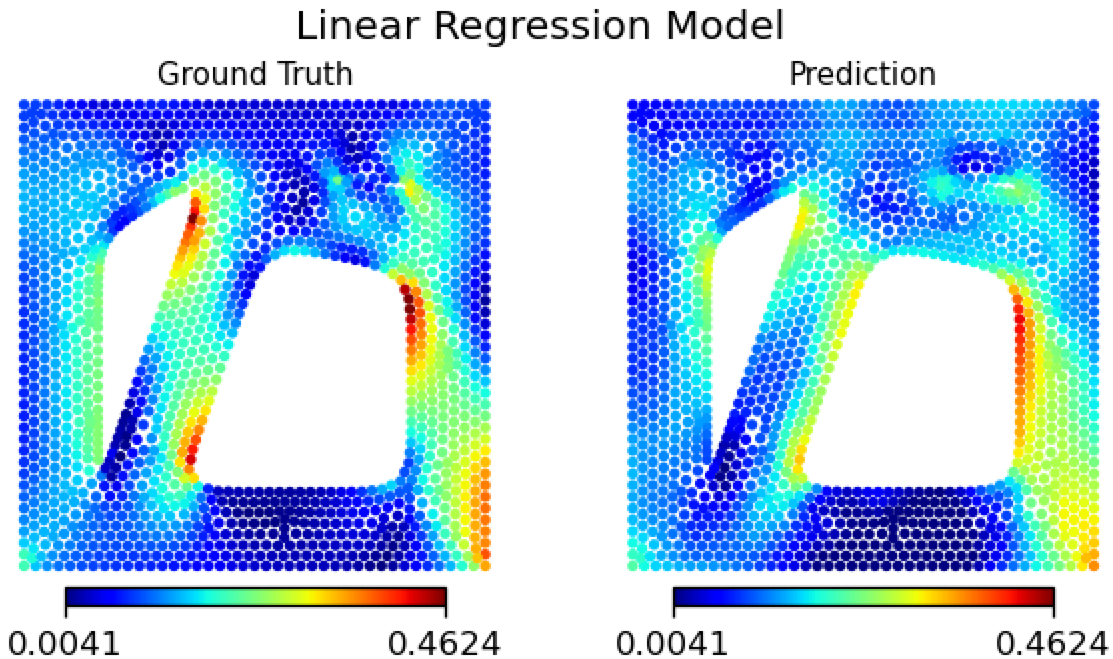
```
Mean squared error for Linear Regression model for the training set: 0.0081106005
Mean squared error for Linear Regression model for the testing set: 0.009779479
Mean squared error for Decision Tree Regressor model for the training set: 0.0004944875978805109
Mean squared error for Decision Tree Regressor model for the testing set: 0.008055742357031064
```

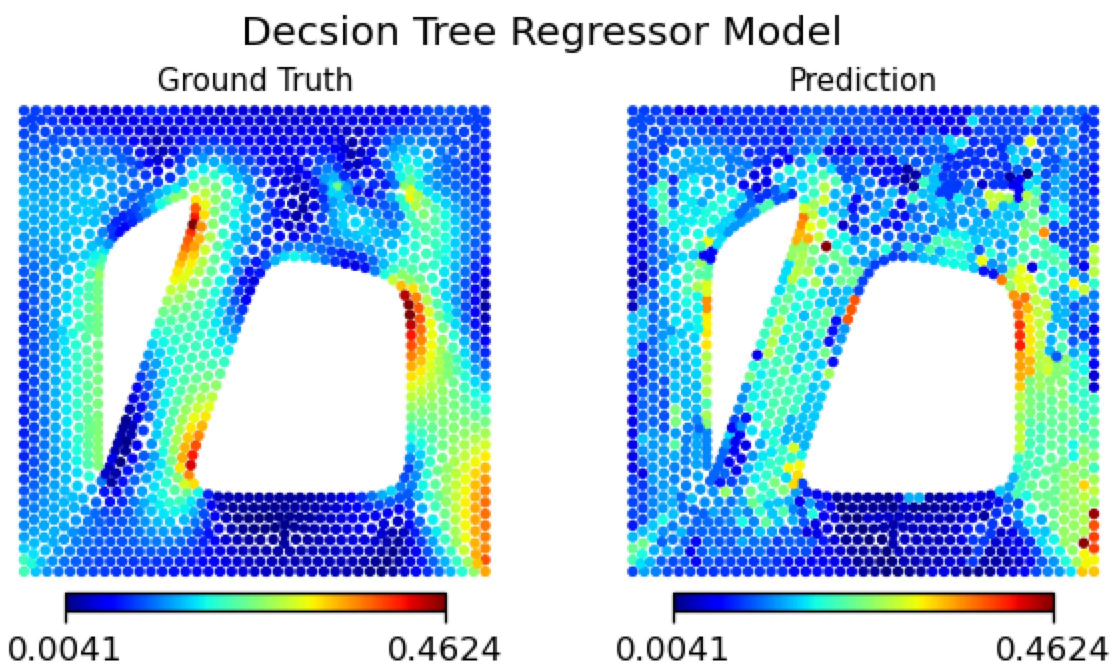
Visualization

Use the `plot_shape_comparison()` function to plot the index 8 shape results in `dataset_test` for each model.

Include titles to indicate which plot is which, using the `title` argument.

In [15]:
```
test_idx = 8
plot_shape_comparison(dataset_test,test_idx,model_lr,title = "Linear Regression Model")
plot_shape_comparison(dataset_test,test_idx,model_dt,title = "Decsion Tree Regressor Model")
# YOUR CODE GOES HERE
```


Linear Regression Model
Ground Truth
Prediction
0.0041
0.4624
0.0041
0.4624

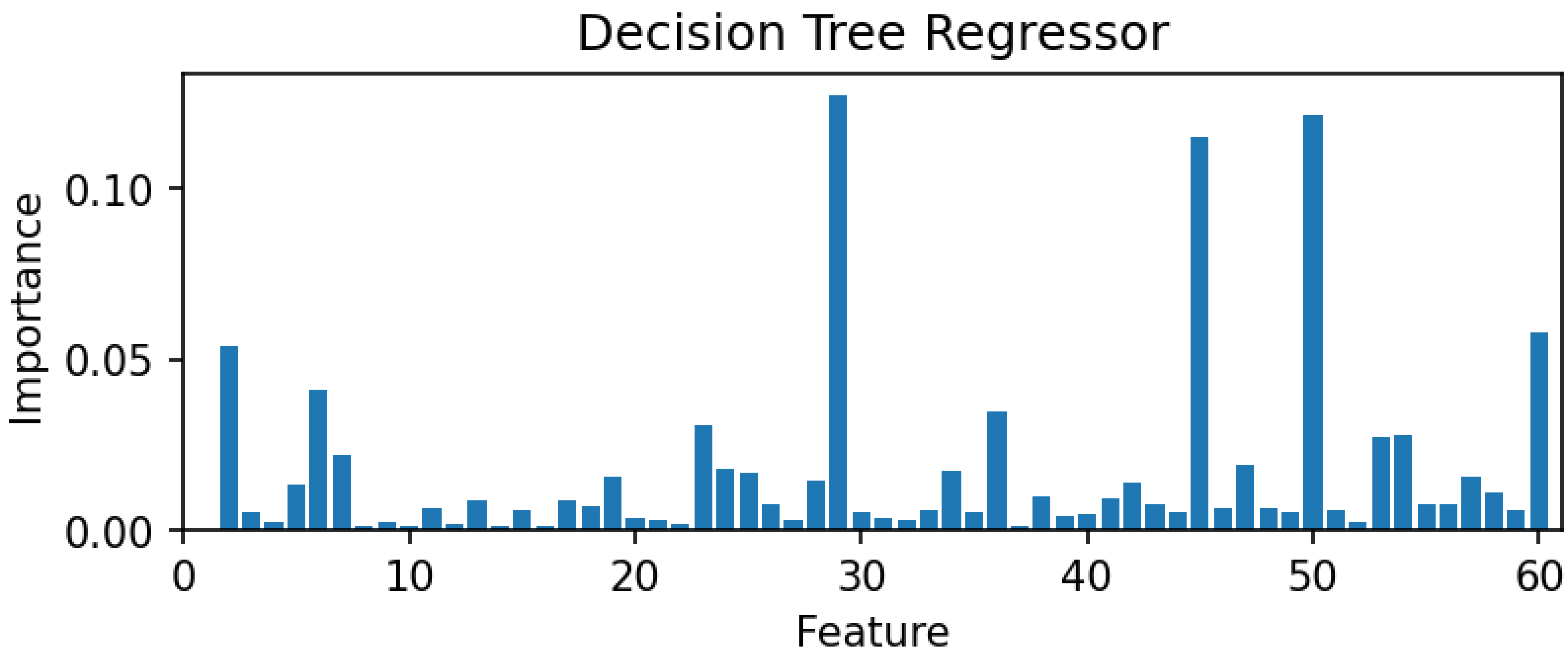

Decsion Tree Regressor Model
Ground Truth
Prediction
0.0041
0.4624
0.0041
0.4624

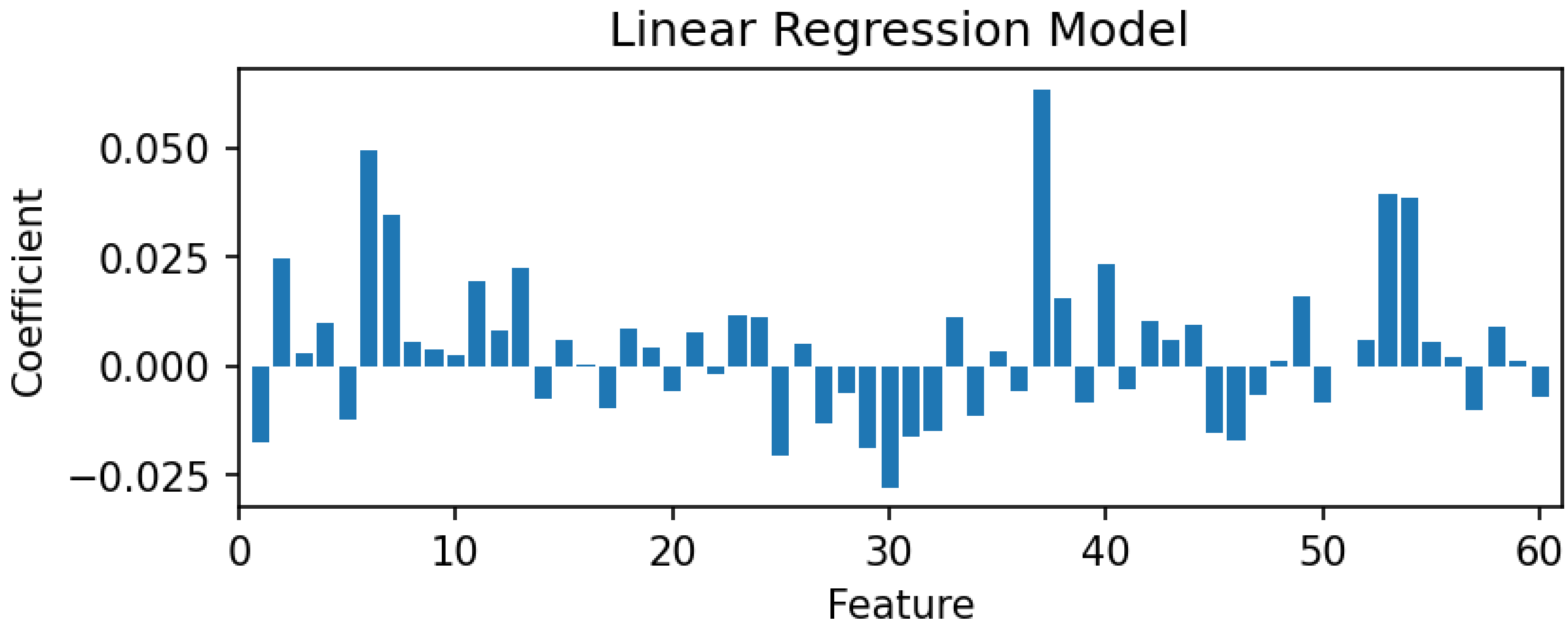
Feature importance

For a tree methods, "feature importance" can be computed, which can be done for an sklearn model using `.feature_importances_`.

Use the provided function `plot_importances()` to visualize which features are most important to the final decision tree prediction. Then create another plot using the same function to visualize the linear regression coefficients by setting the "coef" argument to `True`.

In [16]:
```
# YOUR CODE GOES HERE
plot_importances(model_dt,title="Decision Tree Regressor")
plot_importances(model_lr,coef=True,title="Linear Regression Model")
```





Feature Selection by Recursive Feature Elimination

Using `RFE()` in sklearn, you can iteratively select a subset of only the most important features.

For both linear regression and decision tree (depth 20) models:

1. Create a new model.
2. Create an instance of `RFE()` with `n_features_to_select` set to 30.
3. Fit the RFE model as you would a normal sklearn model.
4. Report the train and test MSE.

Note that the decision tree RFE model may take a few minutes to train.
Visit https://scikit-learn.org/stable/modules/generated/sklearn.feature_selection.RFE.html for more information.

In [17]:
```
# YOUR CODE GOES HERE
model_lr = LinearRegression()
selector = RFE(model_lr,n_features_to_select=30)
selector = selector.fit(X_train,y_train)
```

```
print("Mean squared error for Linear Regression model for the training set:",
      mean_squared_error(y_train,selector.predict(X_train)))
print("Mean squared error for Linear Regression model for the testing set:",
      mean_squared_error(y_test,selector.predict(X_test)))

model_dt = DecisionTreeRegressor(max_depth = 20)
selector_dt = RFE(model_dt,n_features_to_select=30)
selector_dt.fit(X_train,y_train)
print("Mean squared error for Decision Tree Regressor model for the training set:",
      mean_squared_error(y_train,selector_dt.predict(X_train)))
print("Mean squared error for Decision Tree Regressor model for the testing set:",
      mean_squared_error(y_test,selector_dt.predict(X_test)))
```

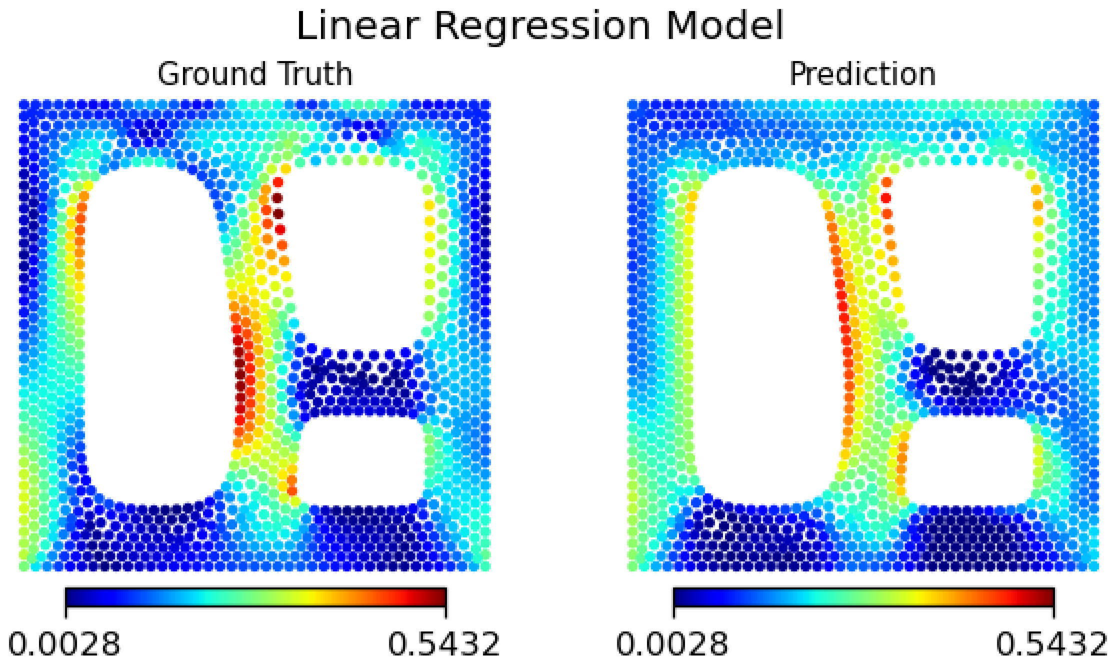
```
Mean squared error for Linear Regression model for the training set: 0.008508719
Mean squared error for Linear Regression model for the testing set: 0.010150377
Mean squared error for Decision Tree Regressor model for the training set: 0.0005573084859188066
Mean squared error for Decision Tree Regressor model for the testing set: 0.009016708176444255
```

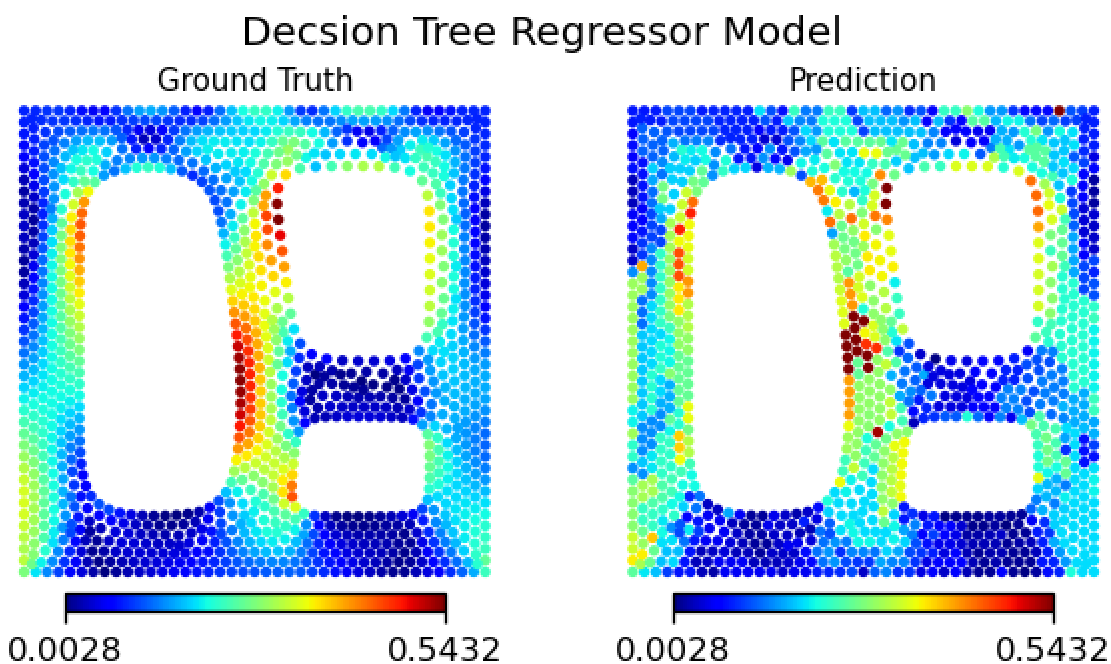
Visualization

Use the `plot_shape_comparison()` function to plot the index 16 shape results in `dataset_test` for each model.

As before, include titles to indicate which plot is which, using the `title` argument.

In [18]:
```
test_idx = 16
plot_shape_comparison(dataset_test,test_idx,selector,title = "Linear Regression Model")
plot_shape_comparison(dataset_test,test_idx,selector_dt,title = "Decsion Tree Regressor Model")
# YOUR CODE GOES HERE
```


Linear Regression Model
Ground Truth
Prediction
0.0028
0.5432
0.0028
0.5432

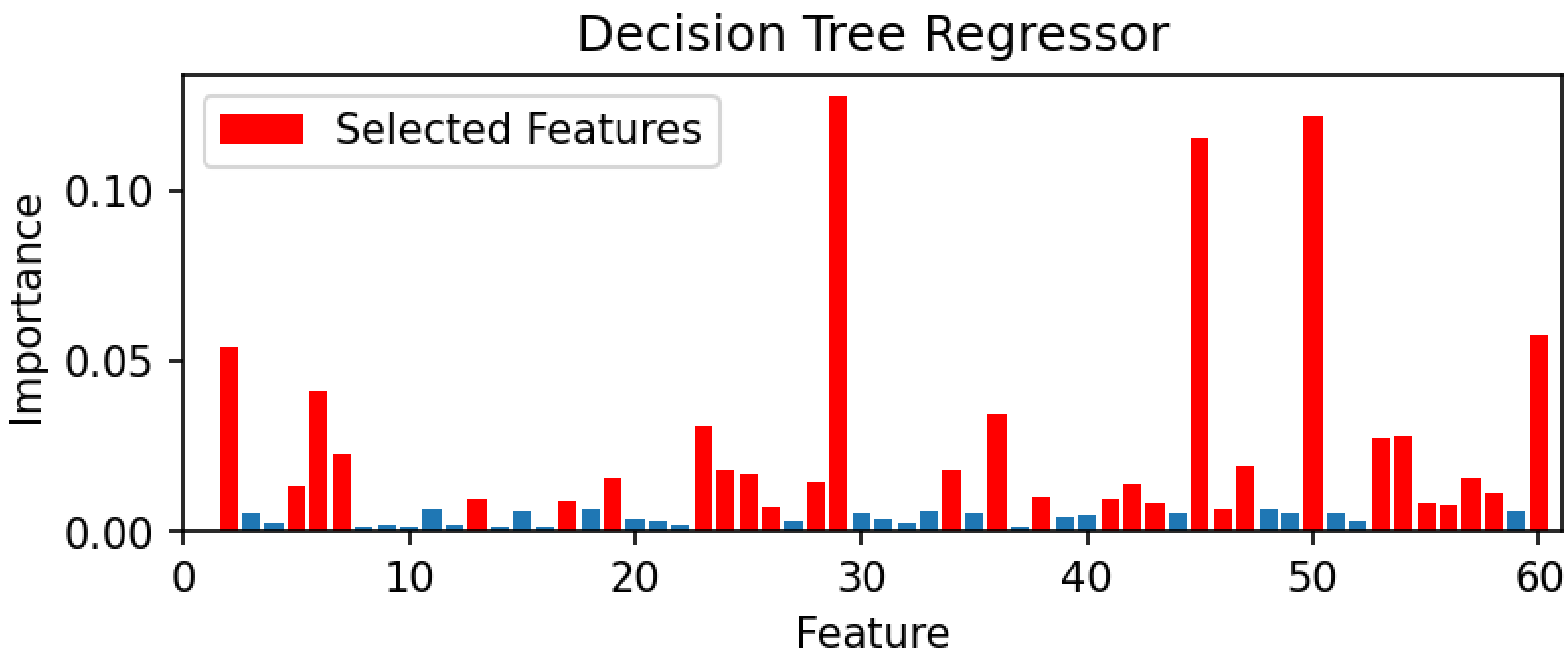

Decsion Tree Regressor Model
Ground Truth
Prediction
0.0028
0.5432
0.0028
0.5432

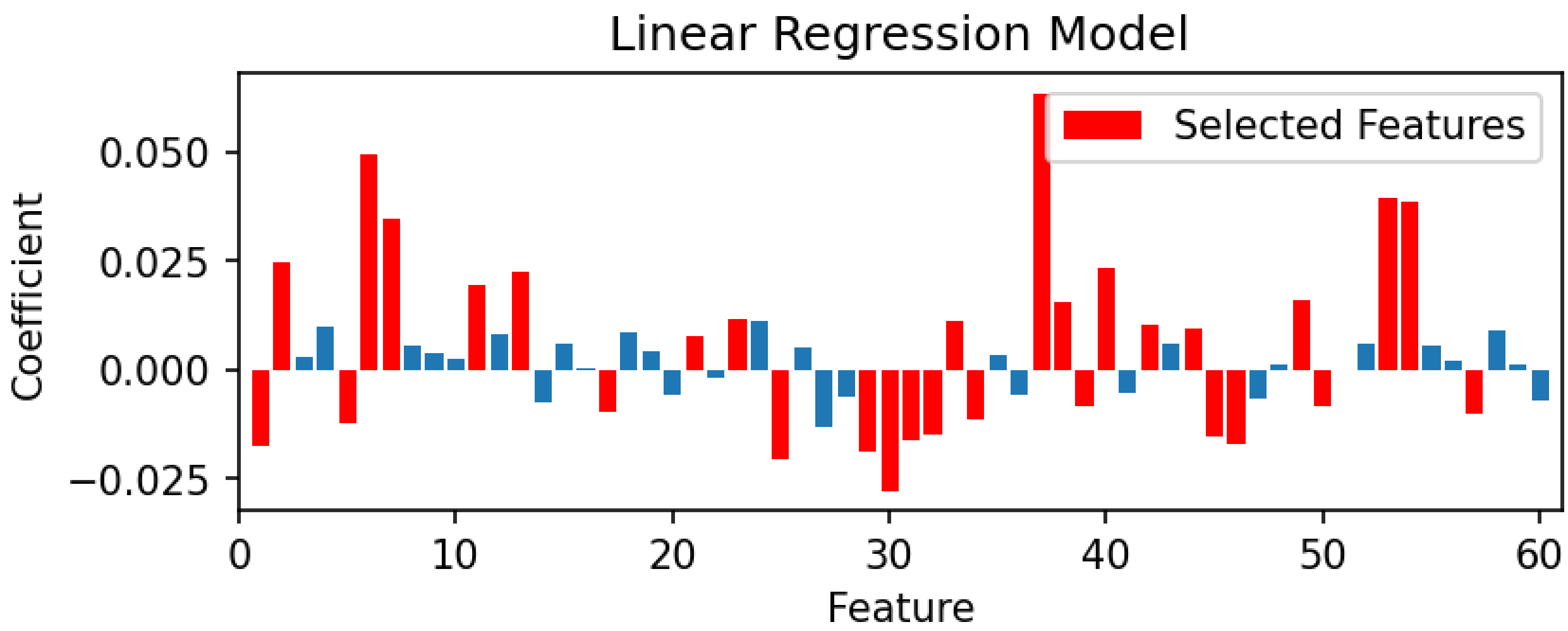
Feature importance with RFE

Recreate the 2 feature importance/coefficent plots from earlier, but this time highlight which features were ultimately selected after performing RFE by coloring those features red. You can do this by setting the `selected` argument equal to an array of selected indices.

For an RFE model `rfe`, the selected feature indices can be obtained via `rfe.get_support(indices=True)`.

In [23]:
```
# YOUR CODE GOES HERE
model_dt.fit(X_train,y_train)
plot_importances(model_dt,selected = selector_dt.get_support(indices=True),title = "Decision Tree Regressor")
model_lr.fit(X_train,y_train)
plot_importances(model_lr,selected = selector.get_support(indices=True),coef=True, title = "Linear Regression Model")
```





Questions

1. Did the MSE increase or decrease on test data for the Linear Regression model after performing RFE?

The MSE increased on test data for the Linear Regression model after performing RFE

1. Did the MSE increase or decrease on test data for the Decision Tree model after performing RFE?

The MSE increased on test data for the Decision Tree Model after performing RFE

1. Describe the qualitative differences between the Linear Regression and the Decision Tree predictions.

The linear regression had a smoother graph as compared to the decision tree prediction. Looking at the graph, the decision tree has more darker blue dots which means that the predictions are lower for decision tree than the linear regression.

1. Describe how the importance of features that were selected by RFE compare to that of features that were eliminated (for the decision tree).

The features selected by RFE has higher importance the features eliminated because the selected features improve the model's performance. The features selected help in making accurate predition than the features that were eliminated. Features selected also split data in the tree that leads to much accurate results. The RFE helps in selecting the features that increase the performance of the model.

1. Describe how the coefficients that were selected by RFE compare to that of features that were eliminated (for linear regression).

The coefficients selected by RFE have a higher importance than the features that were eliminated for linear regression model as the absolute values of the coefficients selected is higher than the ones that were eliminated

In [ ]: